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# Experimental and Theoretical Study of the Electronic and Steric Structure of Seleno- and Thioacetals

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## Abstract

The molecular-orbital and conformational characteristics of a series of seleno- and thioacetals were studied by photoelectron spectroscopy, spectrophotometry of charge-transfer complexes, and PM3 semi-empirical quantum chemical method. The decisive contribution to the HOMO in these compounds is made by the heteroatom bound to the aromatic system, and the characteristics of the second highest occupied molecular orbital depend on the nature of the heteroatoms in the acetal moiety. The stable conformations of the fragments E-CH2-E-CH3 and Ar-Se-CH2-O are trans and gauche, respectively.